
Los Alamos
NATIONAL LABORATORY
EST.1943

Porting EOSPAC6 to Sierra

Anna Pietarila Graham
David Pimentel
Sept 2020

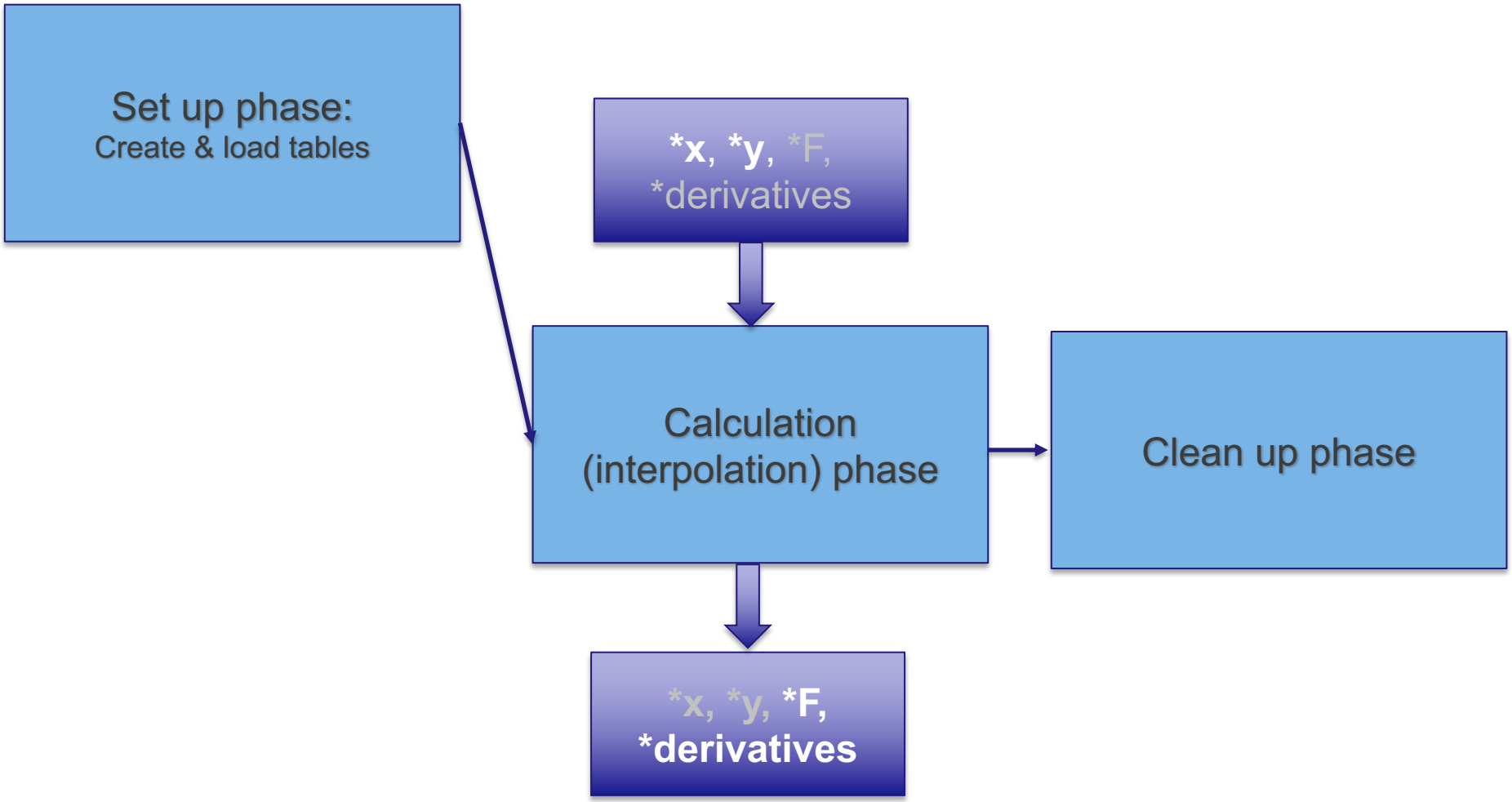
Topics

1. EOSPAC6 Overview
2. Porting goals and strategy
3. Current status and performance
4. Summary and next steps

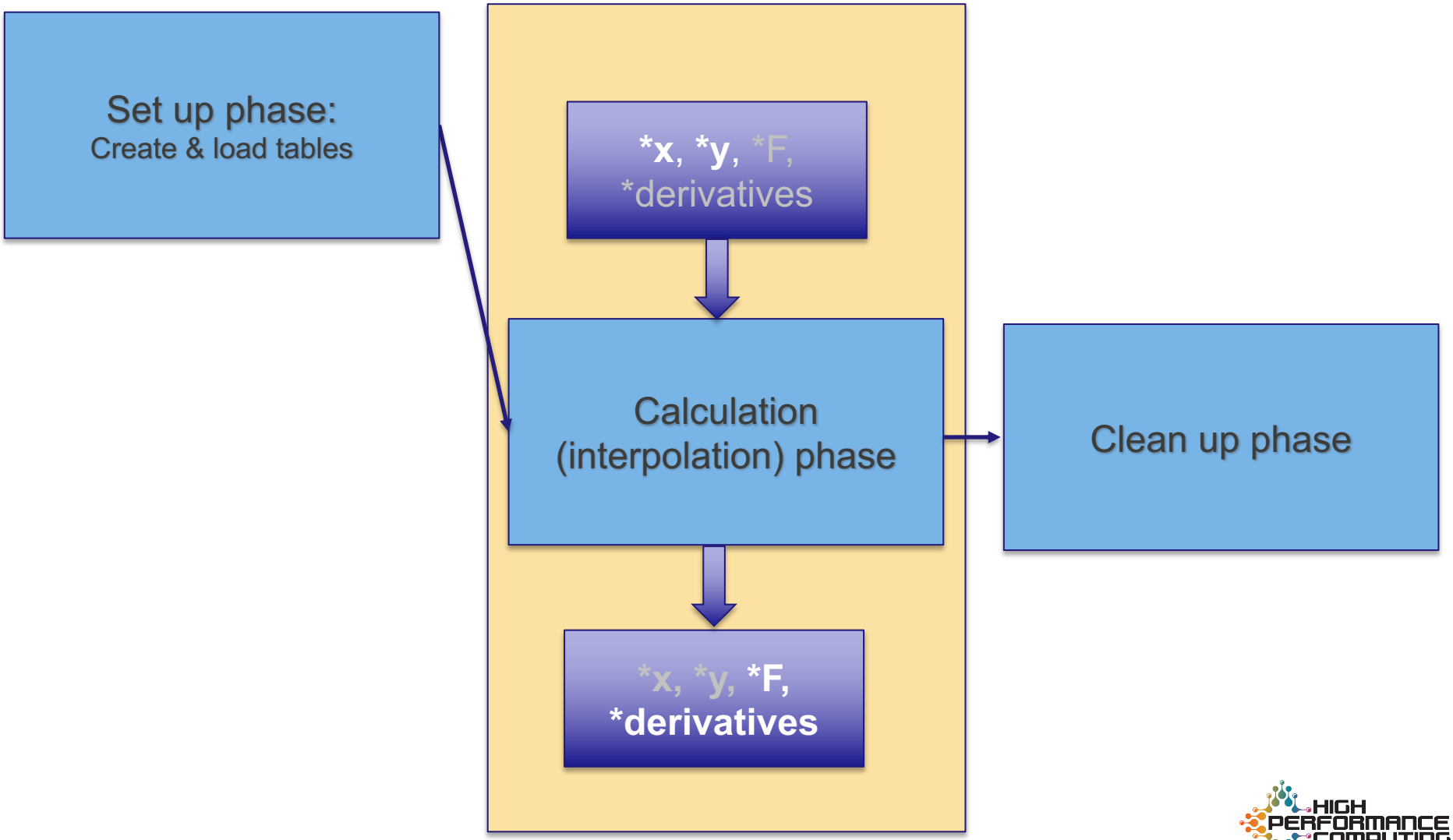
EOSPAC6

- Equation of state library
  - Used to access the Sesame equation-of-state data library and interpolate the data
    - Additional capabilities: mixing, smoothing
  - Development started in 1982, currently at version 6 (2001)
  - Written in C, called from Fortran & C client codes
- Deployed on all LANL HPC systems: 5 compilers, 16 architectures (excluding classified systems)
- Used by multiple large LANL physics codes
- Testing and verification
  - Nightly testing on multiple platforms
  - ~450 regression tests

(Simplified) client code use of EOSPAC6



(Simplified) client code use of EOSPAC6



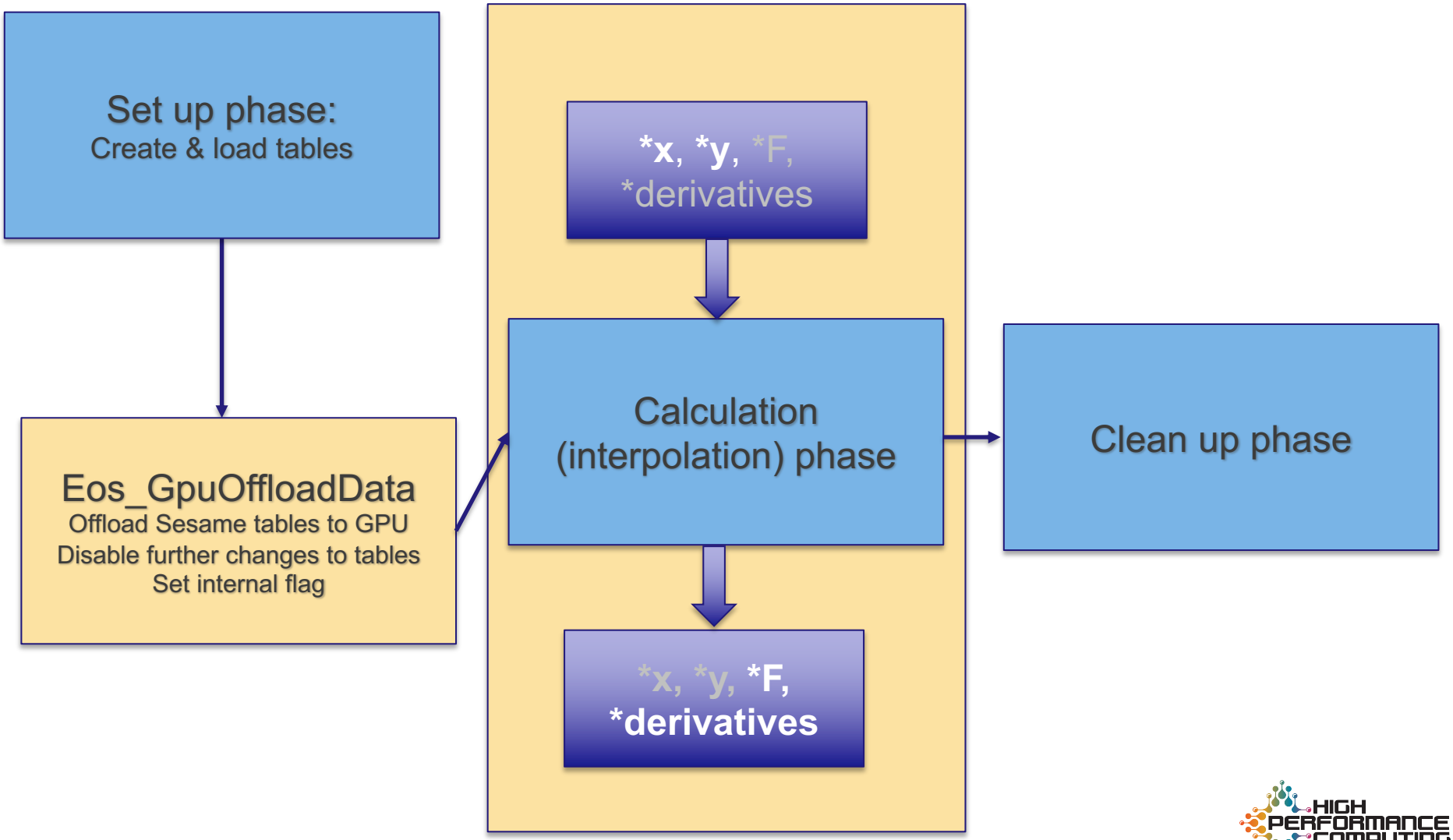
Porting strategy

- From client code point of view:
  - Goal: Most physics computations ported to GPU
  - EOSPAC calls embedded in other code
  - → relevant data already on the GPU

→Work with device pointers as much as possible

  - Minimize data transfers between host and target

(Simplified) client code use of EOSPAC6



Porting strategy

OpenMP offloading

1) Portable & easy to maintain
2) No offload specific kernels need to be written

```
#ifdef DO_OFFLOAD
#pragma omp target if(useGpuData) is_device_ptr(var)
{
#pragma omp teams distribute parallel for
#endif /* DO_OFFLOAD */
```

3) Verification with client code: Shaped charge test setup from Pagosa
   - Representative of typical code path used by client code

- Each client code MPI rank has its own instance of EOSPAC

Current status

- Refactored code e.g.
  - Refactor subroutines to do multiple points instead of single point
  - Rewrite of extrapolated data section
  - Use flat arrays instead of multi-dimensional arrays:

    EOS_REAL *F_flat = !useGpUData?&F[0][0]:&F[0];

- Ported code path used by Pagosa regression test
  - Interpolation & search routines
  - Misc. bits: unit conversion etc.

  - Offloaded code passes tests: EOSPAC6 and Pagosa regression tests

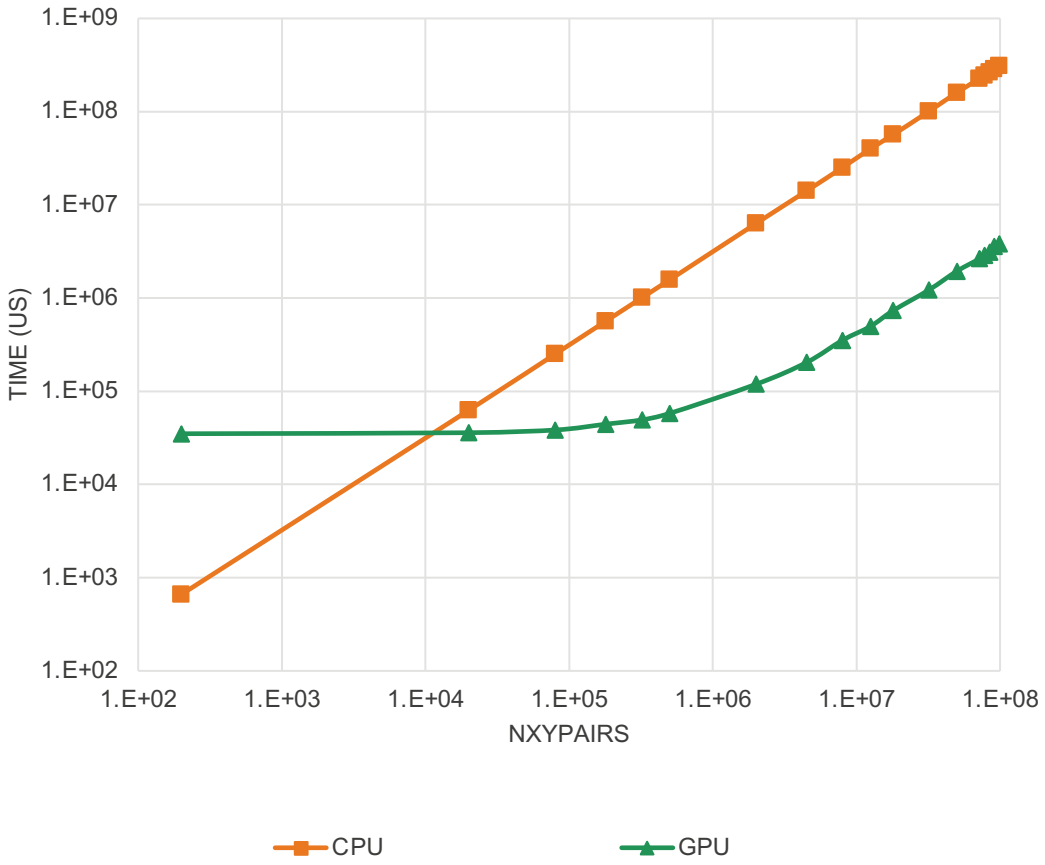
Performance of eos_Interpolate

API called by client code:

void **eos_Interpolate**
(EOS_INTEGER *tableHandle, EOS_INTEGER *nXYPairs,
EOS_REAL *xVals, EOS_REAL *yVals,
EOS_REAL *fVals, EOS_REAL *dFx, EOS_REAL *dFy,
EOS_INTEGER *errorCode);

interpolation & search, bookkeeping, unit conversion,
extrapolation checking (not ported)

Performance: CPU release vs offload



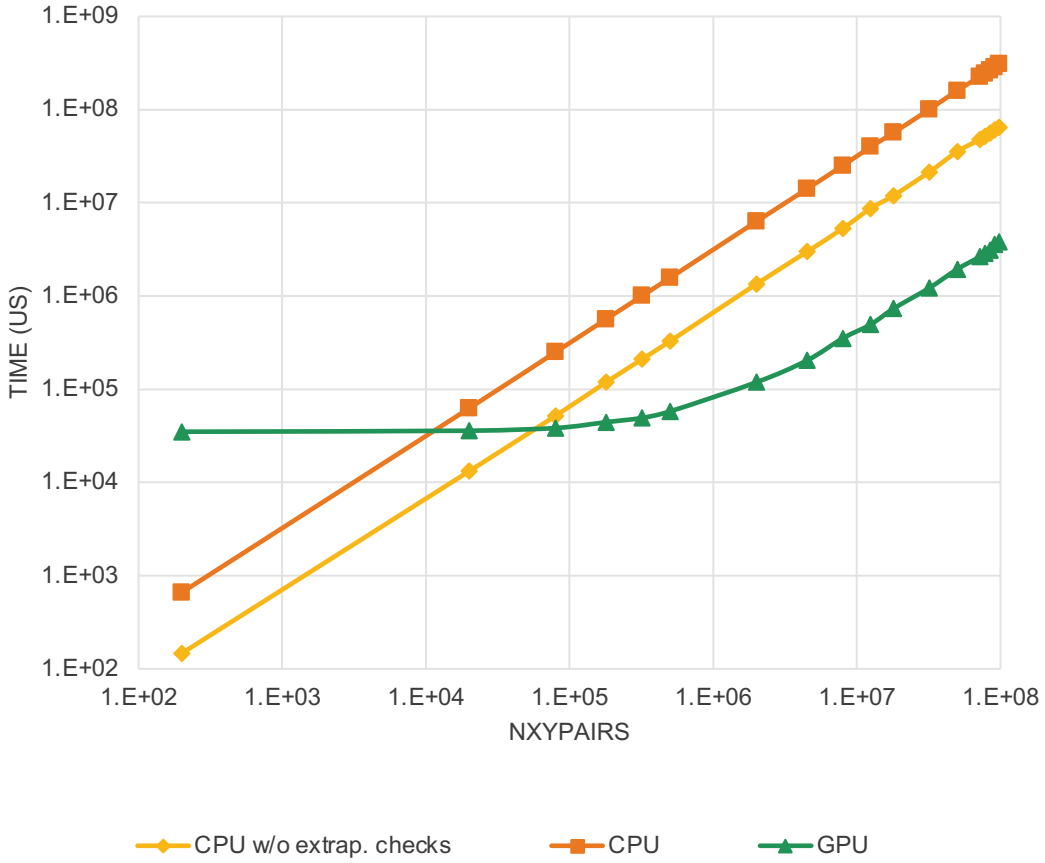
Power9
CPU: serial
GPU: v100

IBM XL
OpenMP 4.5

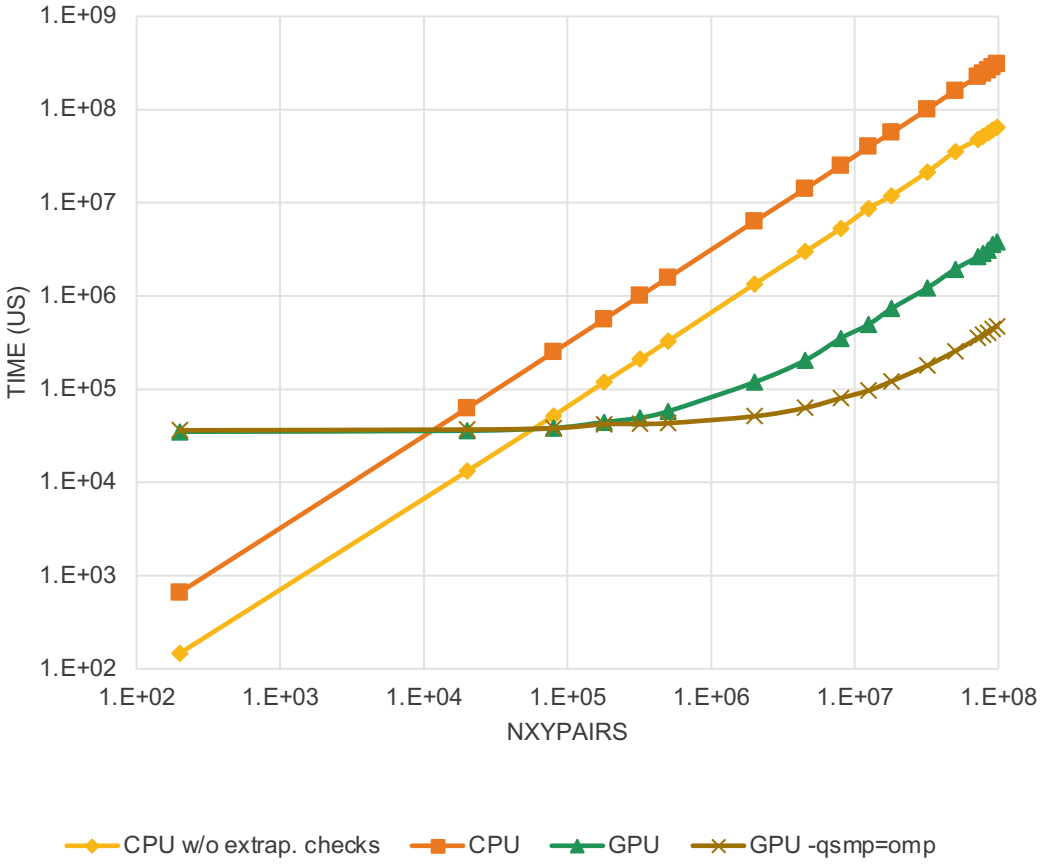
Flags:
-O -qfloat=nomaf
-qstrict=precision

GPU:
-qoffload –qsmp=noopt

Performance: add CPU w/o extrapolation checking

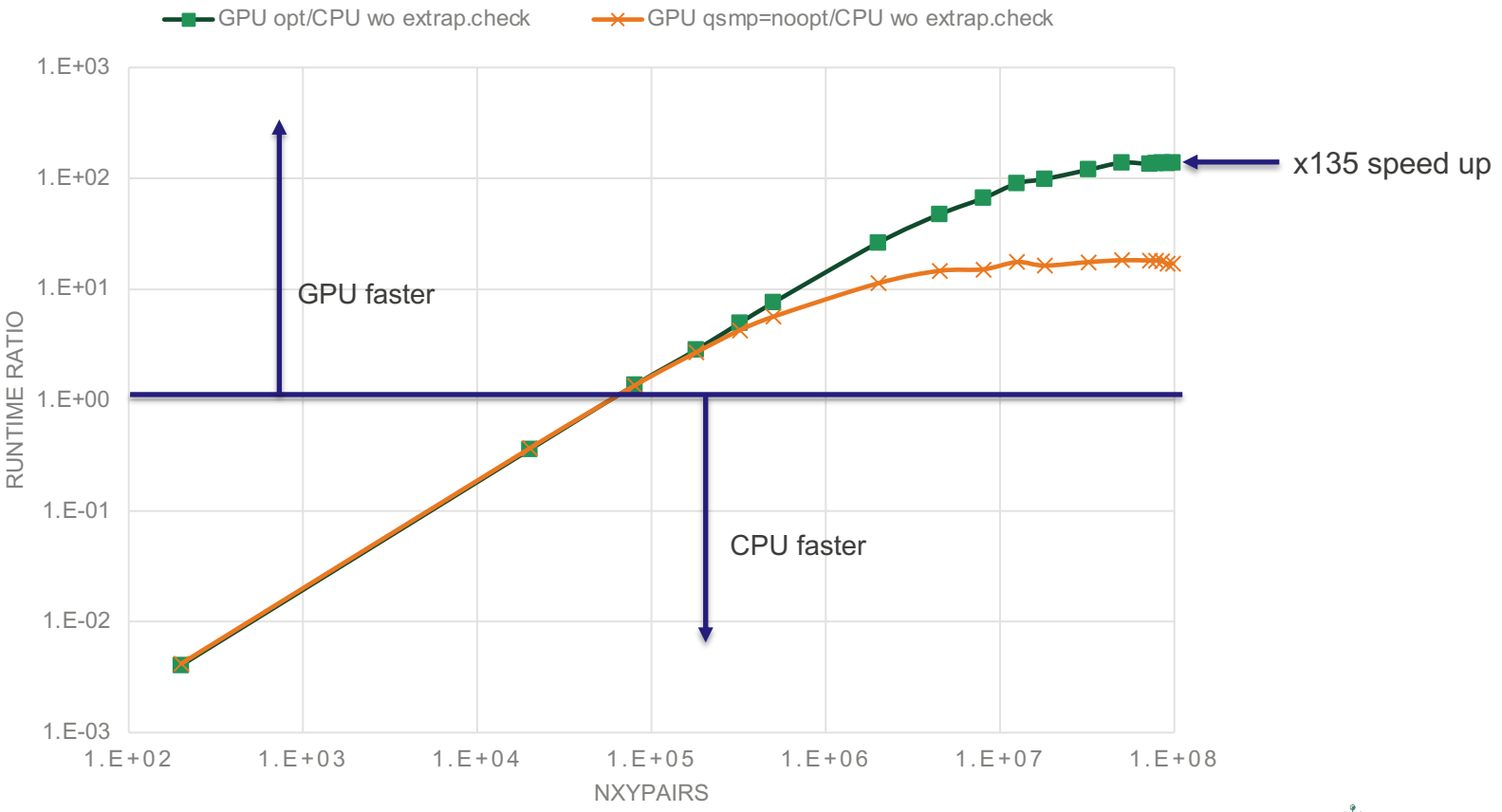


Performance: add optimized offload

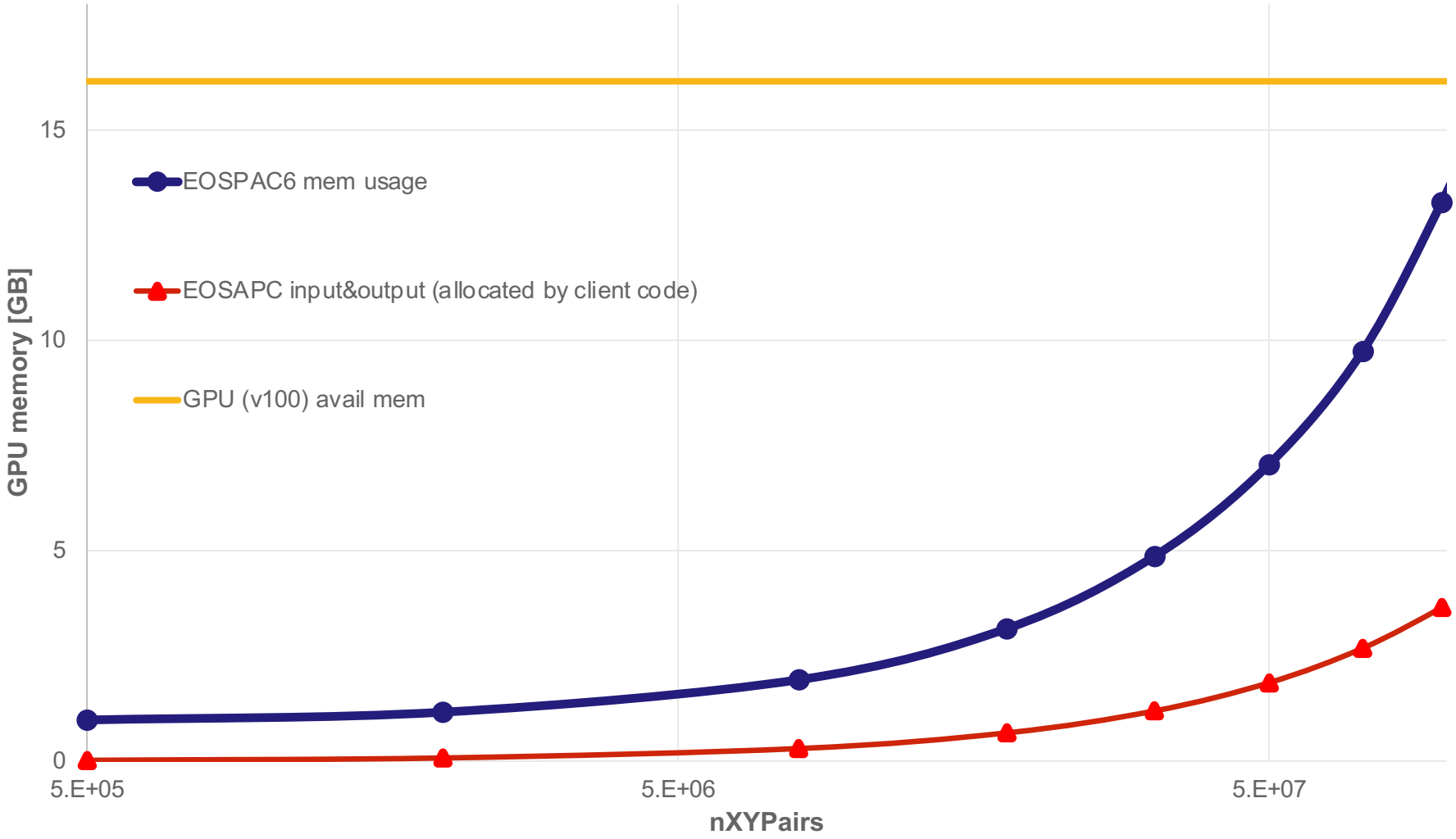


GPU:
-qoffload –qsmp=omp

Performance



EOSAPC6 GPU memory usage (single Sesame table)



Performance bottleneck: extrapolation warnings, error checks (on CPU)

66.79%	313.691s	eos_Interpolate
66.79%	313.691s	| eos_InterpolateEosInterpolation
64.18%	301.421s	| eos_InterpolateRecordType1
64.18%	301.421	| | _eos_InterpolateRecordType1
37.73%	**177.2s**	| | eos_CheckExtrapRecordType1_using_extrapolationBounds
16.72%	78.5102s	| | eos_RationalInterpolateXY
10.49%	49.2501s	| | | _eos_srchdf
8.35%	**39.2101s**	| | | | eos_GetStandardErrorCodeFromCustomErrorCode
4.31%	20.25s	| | | eos_BiRationalInterpolate
8.84%	41.5201s	| | eos_RationalInterpolate
5.35%	25.1501s	| | | _eos_srchdf
4.28%	**20.09s**	| | | | eos_GetStandardErrorCodeFromCustomErrorCode
3.09%	14.52s	| | | eos_RationalInterpolate4

237s of 314s (75%) spent in error and warning code checks

Summary

- Completed proof of concept version using OpenMP offloading
  - Passes validation tests
  - CPU-GPU break-even point: >2. x 10^5 points
  - 135X speed-up when nXYPoints > 10 million
- Identified performance bottle neck in extrapolation checks

Future work

- Port rest of code & create an alpha-release of GPU-enabled library
- Address extrapolation checking
  - New user option to disable checking unless API eos_CheckExtrap is called from client code
- Further performance improvements
  - Temporary array memory usage
  - Optimization of individual kernels
  - …

Over 70 years at the forefront of supercomputing